Projected Dynamics for Metastable Decay in Ising Models

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Abstract. The magnetization switching dynamics in the kinetic Ising model is projected onto a one-dimensional absorbing Markov chain. The resulting projected dynamics reproduces the direct simulation results with great accuracy. A scheme is proposed to utilize simulation data for small systems to obtain the metastable lifetime for large systems and/or for very weak magnetic fields, for which direct simulation is not feasible.

In simulations of metastable decay one faces the problem of measuring the lifetime of the metastable phase, which is by definition very long. For example, in Monte Carlo modeling of magnetization switching in ferromagnets the physically relevant simulation time scales are on the order of $10^{12} - 10^{15}$ Monte Carlo Steps per Spin (MCSS). Even with sophisticated algorithms [1,2] such simulations have not yet been feasible, and one has to resort to extrapolation of the results into the physical time-scale regime.

In this article, a scheme is presented to map the system under study onto a simpler one, which is faster to simulate but still gives accurate results for most important physical quantities. This idea is not new. For example, recently Lee et al. introduced a macroscopic mean-field dynamics [3] which semiquantitatively describes magnetization switching in Ising systems. The aim of the present work is to construct a scheme which is very similar in spirit, but is intended to create a practical computational tool applicable to the simulation of ferromagnets in the physical time regime.

To simplify our notation and reasoning, we explain the proposed Projected Dynamics (PD) as applied to the isotropic kinetic Ising model on a square or cubic lattice. The Hamiltonian has the standard form,

$$\mathcal{H} = -J \sum_{\langle ij \rangle} s_i s_j - H \sum_i s_i \ , \tag{1}$$

with the ferromagnetic nearest-neighbor spin-spin interaction $J > 0$ and an external magnetic field H. In what follows, we denote by V the total number of spins in the system. To study the magnetization reversal, we initialize all spins in the state $+1$, fix the temperature T well below its critical value T_c, and apply

a negative magnetic field. Then we apply Metropolis or Glauber dynamics with updates at randomly chosen sites to measure the time the system needs to reach a configuration with a given stopping magnetization. Repeating this procedure many times, we obtain the mean lifetime, τ, of the metastable state and its standard deviation, $\Delta\tau$.

To speed up the simulations as much as possible, we use a rejection-free algorithm [1,2] which uses the notion of spin classes. By a spin class we mean the state of the spin itself and its neighbors. There are ten classes for the given model on a square lattice. Classes $i = 1, \ldots, 5$ correspond to spins in the state $+1$ which have exactly $i - 1$ neighbors in the state $+1$. Similarly classes $i = 6, \ldots, 10$ are assigned to those -1 spins which have $i - 6$ neighbors in the state $+1$. All spins in class i have the same flipping probability, p_i.

Rejection-free algorithms keep track of the number c_i of spins in each class, and it is not computationally expensive to measure the growth and shrinkage rates of the stable phase, which are defined as

$$g(n) = \sum_{i=1}^{5} \langle c_i \rangle_n p_i \quad , \quad s(n) = \sum_{i=6}^{10} \langle c_i \rangle_n p_i \ , \tag{2}$$

respectively. The angular brackets mean the average taken over the configurations generated during the Monte Carlo lifetime experiment, conditionally on the number n of overturned spins. Thus, $g(n)/V$ is the probability that a $+1$ spin will be flipped in the next Monte Carlo step, and $s(n)/V$ is the probability to flip one of the -1 spins, both conditionally on n. Flipping a $+1$ spin increases the volume fraction of the stable phase, hence the names $g(n)$ and $s(n)$.

The main idea of the proposed method is to make use of the observed growth and shrinkage rates to map the switching dynamics onto a one-dimensional absorbing Markov chain. We assign to all configurations with n overturned spins a single state n in the chain. The one-dimensional dynamics is given by the above probabilities: From the state n we have the probability $g(n)/V$ of jumping to the state $n + 1$, the probability $s(n)/V$ of jumping to $n-1$, and the probability $1-g(n)/V-s(n)/V$ of remaining in the current state. This random walk starts at $n = 0$ and terminates when it reaches $n = N + 1$ where $M = V - 2N - 2$ corresponds to the stopping magnetization. Using standard methods from the theory of absorbing Markov chains [2,3], we obtain the mean lifetime τ and the total average time $h(n)$ (in MCSS) spent by the random walker in the state n in terms of the growth and shrinkage rates:

$$\tau = \sum_{n=0}^{N} h(n) \quad , \quad h(n) = \frac{1 + s(n+1)h(n+1)}{g(n)} \quad , \quad h(N) = \frac{1}{g(N)} \ . \tag{3}$$

Higher moments of the lifetime distribution can be obtained in a similar way.

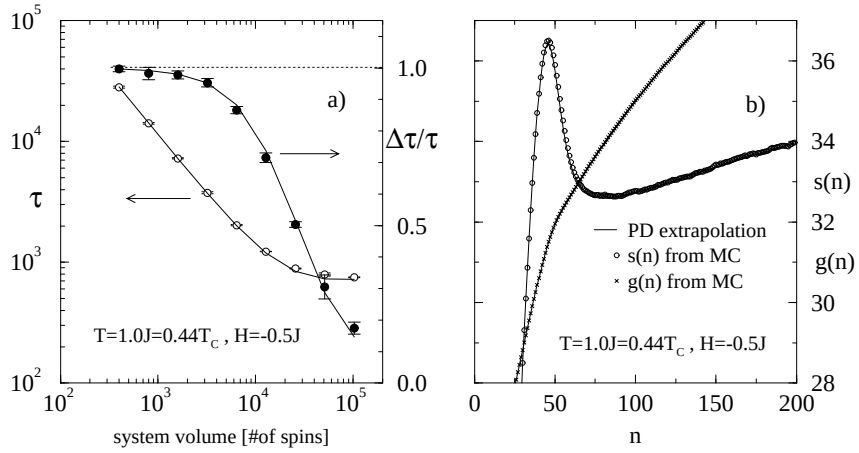

Fig. 1 Illustration of the Projected Dynamics [Eqs. (2,3)] and of the "size extrapolation" scheme [Eq. (4)]. The lines in both panels are Projected Dynamics extrapolations based on $\langle c_i \rangle_n$ sampled during lifetime measurements on a 20×20 lattice. Symbols are direct simulation results. a) The lifetime and its relative standard deviation vs. the system volume. The agreement is near-perfect in the single-droplet regime (where $\Delta\tau/\tau \approx 1$), and deviations are only observed in the crossover region to the multidroplet regime (where $\Delta\tau/\tau \to 0$). b) Extrapolation from the 20×20 lattice reproduces the measured growth and shrinkage rates, $g(n)$ and $s(n)$, of the 160×160 lattice very well. The crossings of the two curves correspond to the metastable magnetization (left) and the critical fluctuation (right).

As shown in Fig. 1, the proposed scheme reliably reproduces the direct Monte Carlo results. The lifetimes obtained from Eq.(3) are usually only slightly different from their counterparts from the direct measurements. The projected dynamics also gives the standard deviation of the lifetime distribution, which agrees with the measured values within the error bars.

Suppose we have measured $g(n)$ and $s(n)$ in a system of volume V. How are they related to their counterparts in a system of volume $2V$? Since the relevant configurations typically contain many small droplets of the stable phase, it is a reasonable approximation to view the larger system as consisting of two "independent" copies of the smaller system. Then, the growth rate of the large system can be approximated as a weighted sum of the sub-system contributions,

$$g(2V,n) \approx \frac{\sum_{i=0}^{n} h(V,n-i)h(V,i)[g(V,n-i)+g(V,i)]}{\sum_{i=0}^{n} h(V,n-i)h(V,i)} \; . \qquad (4)$$

Here, we have explicitly shown the dependence on the volume V. An analogous formula is proposed for the shrinkage rate $s(n)$. Provided the smallest system is in the so-called single-droplet regime, in which the nucleation is triggered

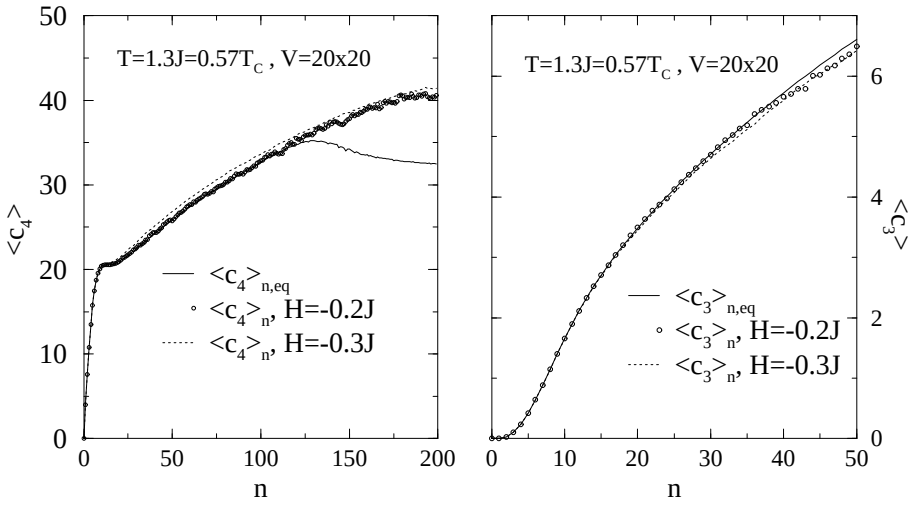

Fig. 2 Populations of two spin classes vs. the number of overturned spins n. Solid lines are $\langle c_i \rangle_{n,\mathrm{eq}}$ measured in the equilibrium fixed-n ensemble; circles and dotted lines show $\langle c_i \rangle_n$ measured during the lifetime measurement for two different fields. Note that as the field decreases the region in which $\langle c_i \rangle_n \to \langle c_i \rangle_{n,\mathrm{eq}}$ increases.

by a single critical fluctuation smaller than the system size (for the theoretical description of different regimes of the magnetization switching, see Refs. [4-8]), one can repeat the extrapolation $V \to 2V$ several times without finding a big discrepancy between growth and shrinkage rates calculated from the small-lattice data and those directly measured on large lattices (see Fig. 1b).

Now we return to our main goal, namely predicting lifetimes in very weak fields. What we need is to calculate $g(n)$ and $s(n)$ as functions of the magnetic field. The naive choice would be to replace the class spin-flip probabilities p_i by their values calculated for the desired field, and keep the values $\langle c_i \rangle_n$ entering Eq. (2) unchanged. Such a scheme works quite well when extrapolating to stronger fields, but the lifetimes are systematically overestimated for fields weaker than the one at which the $\langle c_i \rangle_n$ were sampled. The reason lies in the nonequilibrium character of the configurations with n larger than the critical droplet volume (see Fig. 2). As it tries to escape from the metastable free-energy minimum, when n is small the system passes through configurations which are very close to "equilibrium". Farther from the free-energy minimum, the configurations which appear in the system are increasingly different from "equilibrium" configurations. Although these configurations do not contribute significantly to the lifetime, if we use them to estimate the lifetime in a *weaker* field their contribution becomes more important because the system then spends more time in them. However, the actual configurations are closer to "equilibrium," because the free-energy minimum is deeper in a weaker field.

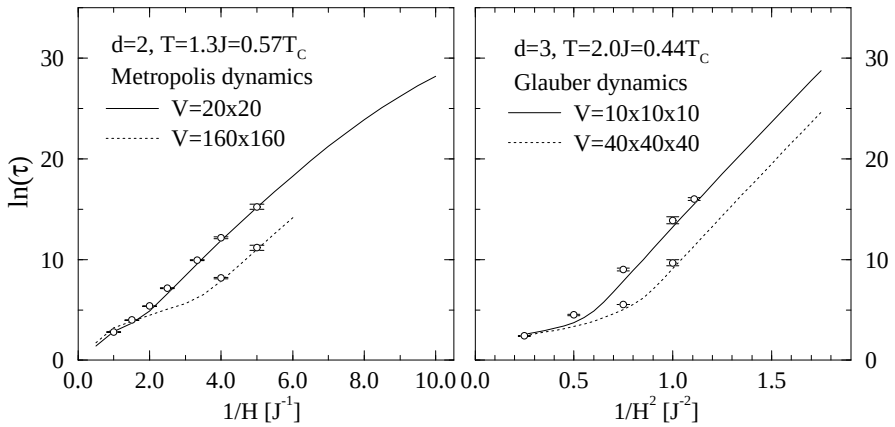

Fig. 3 The metastable lifetime of a kinetic Ising model as a function of the magnetic field. Points are conventional Monte Carlo measurements, and lines are Projected Dynamics calculations based on the "equilibrium" $\langle c_i \rangle_{n,\mathrm{eq}}$ data sampled on the smaller systems. Predictions of the Projected Dynamics improve with decreasing field.

Thus, we effectively replace the actual weak-field configurations by ones which appear slightly "overheated." This enhances the shrinkage probabilities more than the growth probabilities, thus leading to an overestimate of the metastable lifetime. Understanding the cause of this problem also offers a remedy: we can do better by using the equilibrium configurations. Then we expect to see underestimation of relatively short lifetimes (by reversing the above argument). On the other hand, such an approximation will improve with decreasing field, which is exactly what we need to extrapolate towards zero field. Thus, we define the equilibrium growth and shrinkage rates as follows

$$g_{\mathrm{eq}}(n) = \sum_{i=1}^{5} \langle c_i \rangle_{n,\mathrm{eq}} p_i \quad , \quad s_{\mathrm{eq}}(n) = \sum_{i=6}^{10} \langle c_i \rangle_{n,\mathrm{eq}} p_i \ . \tag{5}$$

The only difference from Eq. (2) is in the sampling. Here, $\langle c_i \rangle_{n,\mathrm{eq}}$ are sampled in an equilibrium ensemble with a fixed number of overturned spins n. Thus, instead of sampling the configurations during the lifetime measurement, we perform a static measurement for each value of n needed (up to the stopping magnetization). The $\langle c_i \rangle_{n,\mathrm{eq}}$ depend on temperature, but the only dependence of g_{eq} and s_{eq} on the magnetic field comes from the spin-flip probabilities p_i. In that way, a single measurement provides sufficient data to obtain a good approximation for the lifetime as a function of the external field.

Figure 3 shows the lifetime calculated from the projected dynamics for two pairs of lattice sizes in two and three dimensions. Comparison with the direct simulation results (points) corroborate our expectation that the lifetime

is underestimated in the crossover region between the single-droplet and multidroplet regimes, and that the approximation provides progressively better results as the external field strength decreases. Measurements on small lattices, for which we can obtain reasonable statistics in zero field, show that the Projected Dynamics based on $\langle c_i \rangle_{n,\mathrm{eq}}$ reproduces the "lifetime" in zero field.

In conclusion, our Projected Dynamics maps the complex Monte Carlo dynamics onto a much simpler one-dimensional absorbing Markov chain. The Projected Dynamics is computationally much easier to study than the full underlying Monte Carlo dynamics, while it provides reliable results for metastable lifetimes and their standard deviations. Data from small systems can be utilized to predict lifetimes for large systems. When based on "equilibrium" class populations $\langle c_i \rangle_{n,\mathrm{eq}}$, Projected Dynamics yields results as functions of the field. Such estimates are most reliable in the experimentally relevant weak-field region, which it is currently not feasible to investigate with direct simulations. The method also offers a deeper insight into the mechanism of metastable decay. For example, the histogram $h(n)$ provides a simple method to measure the metastable magnetization and susceptibility, and the rates $g(n)$ and $s(n)$ contain information about the size of the critical fluctuations.

For other types of models, the applicability of the projected dynamics will depend on the existence of a "single channel" for the decay. The projected parameter (n in the present case) need not necessarily be related to the magnetization, but it should parameterize the optimal path for escape from metastability in such a way that the configurations at a fixed value of the parameter will exhibit similar growth and shrinkage rates.

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References

[1] A. B. Bortz, M. H. Kalos and J. L. Lebowitz, J. Comput. Phys. **17**, 10 (1975).
[2] M. A. Novotny, Phys. Rev. Lett. **74**, 1 (1995); Erratum **75**, 1424 (1995).
[3] J. Lee, M. A. Novotny and P. A. Rikvold, Phys. Rev. E **52**, 356 (1995).
[4] P. A. Rikvold, H. Tomita, S. Miyashita and S. W. Sides, Phys. Rev. E **49**, 5080 (1994).
[5] H. L. Richards, S. W. Sides, M. A. Novotny, and P. A. Rikvold, J. Magn. Magn. Mater. **150**, 37 (1995).
[6] H. L. Richards, S. W. Sides, M. A. Novotny, and P. A. Rikvold, J. Appl. Phys. **79**, 5479 (1996).
[7] H. L. Richards, M. A. Novotny, and P. A. Rikvold, Phys. Rev. B **54**, 4113 (1996).
[8] H. L. Richards, M. Kolesik, P.-A. Lindgård, P. A. Rikvold, and M. A. Novotny, Phys. Rev. B, **55** in press.